Teaching SEMIPHYSICAL MODELING to ChE Students Using a Brine-Water Mixing Tank Experiment

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Process dynamics education in the ChE curriculum is usually accomplished as part of a dedicated controls course, which is listed in most programs of study as a senior-year course; many papers have been published in the literature describing process control educational efforts and laboratories.[1-3, 5, 8] The fundamentals of the dynamical behavior of engineering systems can be adequately presented much earlier in the curriculum, however, and done so in the context of applications more general than process systems. Including a laboratory experience as part of this instruction provides an opportunity for students to develop analysis skills as well as a working feel for abstract concepts that will prove valuable in later courses and during their subsequent careers.

Such an experience was provided to chemical engineering students at Arizona State University. "Understanding Engineering Systems via Conservation," (ECE 394 Systems) was the third in an experimental core curriculum developed at Texas A&M[4] which was part of the chemical engineering curriculum at ASU from 1992 to 2003. Students traditionally took ECE 394 Systems in the spring semester of their junior year. This four-credit-hour course was structured with three lecture hours a week and one weekly two-hour recitation. The course stressed the broad-based use of accounting and conservation principles to model systems involving process, electrical, and mechanical components (separately and in combination). Another principal course objective was the use of computer-based tools to model engineering systems of practical interest.

In ECE 394 Systems, students were confronted with the "reality" of engineering systems from the very first lecture. Students are made aware that most real systems are

- ***Dynamic/unsteady-state*** *("steady-state is a figment of the imagination")*
- ***Nonlinear***
- ***Multivariable*** *(i.e., possessing multiple inputs and outputs)*

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- ***Uncertain*** *(i.e., models of real systems lack accuracy)*
- ***Stochastic*** *(i.e., real systems are subject to random behavior, and as such cannot be always described by deterministic models; precision errors will always be present in models)*

Starting in the first lecture (and frequently thereafter) students were also presented with the saying attributed to famous statistician Prof. G.E.P. Box of the University of Wisconsin, "All models are wrong, but some are useful."

Students in the course work in recitation as part of three-person teams. Two individual reports and three group presentations are required as part of the modeling project.

The brine-water tank experiment (Figure 1) was used in ECE 394 Systems as an ongoing project to indoctrinate students to reconciling the abstraction of mathematical modeling with the realities of a practical system. The main objective of this experiment is to develop — via first principles and semiphysical modeling techniques — *useful* mathematical models of the tank behavior displaying good predictive ability. Specifically, the students are asked to model the dynamic response of salt concentration in the outlet stream (c) and level in the tank (h) to changes in the inlet brine flowrate (q_c), the freshwater flowrate (q_w), and outlet flow (q_F). The tank is interfaced to a industrial-scale, real-time computing platform, namely a Honeywell TotalPlant Solution System (previously known as the TDC3000, Figure 2). The engineer is capable of adjusting all three tank flows via the TDC3000 regulatory control points FIC100, FIC101, and LIC100 (see Figure 1). The experiment also requires students to generate a suitable calibration between the signal generated from an online conductivity sensor and the salt concentration (in g/ℓ) for the outlet stream in the tank.

This paper describes the following aspects of the project:

- *The experimental apparatus*
- *The first-principles model for the tank and the corresponding derivation of a semiphysical model for this system*
- *The steps involved in developing a comprehensive semiphysical modeling procedure, beginning with experimental design and concluding with model validation; the procedure is illustrated with actual experimental data obtained from the tank*
- *Recommendations for the use of this experiment in other courses in the ChE curriculum*

EXPERIMENTAL DESCRIPTION

Figure 1 shows both the process and the instrumentation used in this experiment. The flow of tap water to the process is regulated by measuring the flow with an orifice meter and changing the valve position on the water line according to an algorithm in a regulatory control point in the TDC3000. This control loop is assigned the tagname FIC100. Similarly, the flow of a concentrated salt solution is controlled with loop FIC101. The level in the tank is measured with a differential pressure cell (d/p) with one leg connected to the bottom of

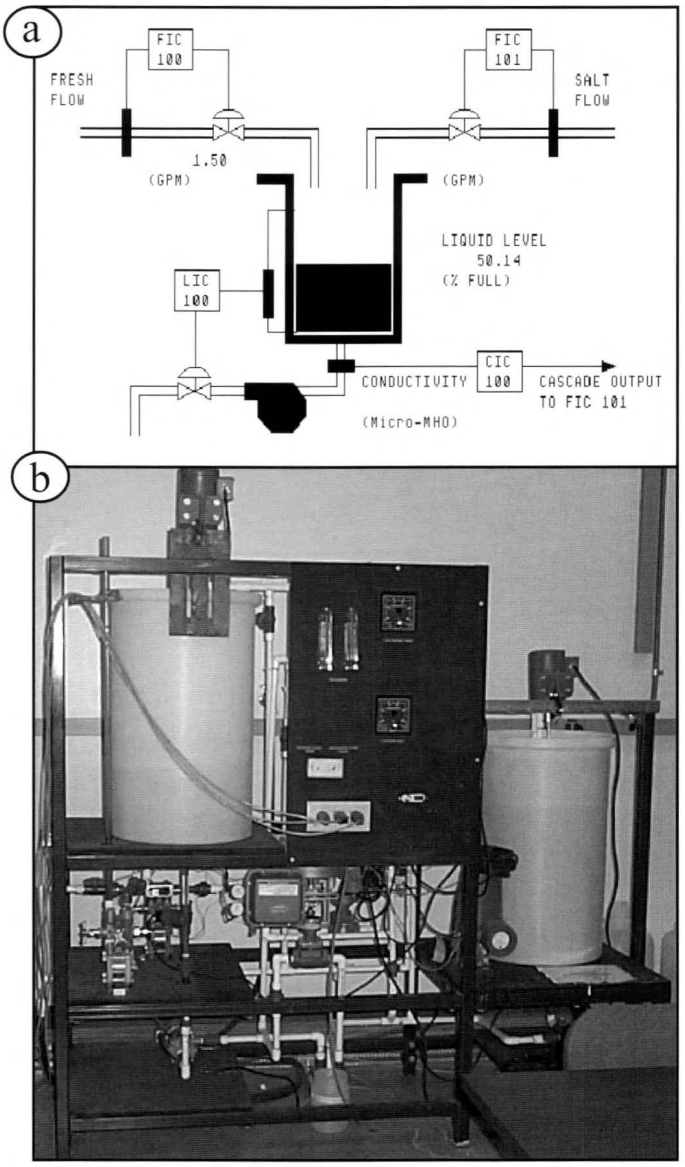

Figure 1. *The brine-water mixing tank in diagram* ***(a),*** *and pictured* ***(b).***

Figure 2. *Representative cluster of Universal and Global User Stations for ASU's TotalPlant Solution System.*

the tank and the other leg open to the atmosphere. The regulatory control point LIC100 compares this level with a desired level and manipulates the flow through the drain line. The salt concentration leaving and entering the tank is measured with conductivity cells and is read into the system via analog input points CI100 and CI102, respectively. The conductivity measurements are displayed as the PVs (process values) of CI100 and CI102. By setting the appropriate instrument range-limit parameters in the system (*e.g.*, PVEUHI and PVEULO) the students are able to implement a linear correlation relating the raw 4-20ma signal from the conductivity cells to a sensible value for concentration in units of g/ℓ.

CIC100 is a regulatory control point used in a subsequent course (ChE 461, Introduction to Process Control[7]) which adjusts the salt-inlet flowrate setpoint (FIC101.SP) to keep exit-stream salt concentration at setpoint (CI100.PV); students are asked to leave this point on "manual" throughout the experiment.

The mixing tank experimental apparatus has been a long-standing fixture of the undergraduate chemical engineering laboratories at ASU, having been in continuous use since the mid-1980s. The cost to build a system of similar size to the one shown in Figure 1 (not including the data acquisition and control equipment) is estimated at slightly more than $8,000. This total is roughly broken down into the following: $200 for two polypropylene tanks, $4,000 for sensors (consisting of two flow meters, three differential pressure cells, and two conductivity cells with transmitters), $3,600 for three electro-pneumatic valves, and $350 for the rack/frame and associated piping and wiring. Once built, the experiment requires only basic maintenance for adequate operation; since 1990 our setup has only required replacing the polypropylene tanks and one of the conductivity transmitters.

The TDC3000/TotalPlant Solution System is also a long-standing fixture of our laboratory (having been donated by Honeywell to our program in 1990, as described in Reference 7). But, in lieu of a commercial distributed-control system, a readily available data acquisition platform such as LabVIEW from National Instruments (<http://www.ni.com>) can be used as a computer interface with the system. We should note that a smaller-scale apparatus can be used to accomplish the experiment described in this paper; for example, the bench-scale brine-water tank experiment described by Bequette and Ogunnaike[2] could readily be adapted for the purposes here.

BRINE-WATER TANK MODELING

First-Principles Modeling

During lecture and through homework assignments, students use Matlab with Simulink to develop a first-principles dynamical model describing the effect of the various system inputs on the level and salt concentration. The principles of conservation of total mass and accounting of the salt species in the tank are used to derive this model. The level dynamics of the system are described by a differential equation arising from the conservation of total mass in the system

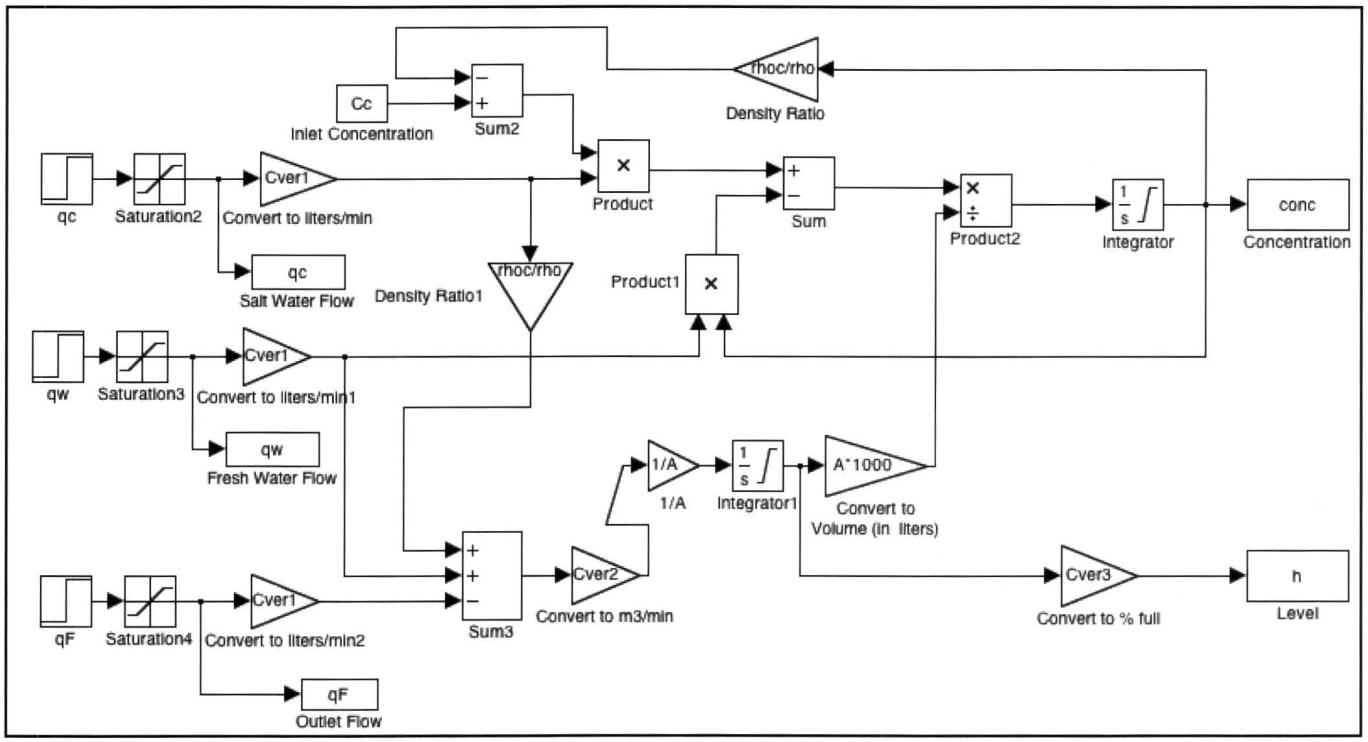

Figure 3. *Simulink window for the brine-water mixing tank first-principles model.*

$$\frac{dh}{dt}=\frac{1}{A}\left(q_w-q_F+\frac{\rho_c}{\rho}q_c\right) \tag{1}$$

while the dynamics of salt in the tank are modeled by accounting for this species in the system

$$\frac{dc}{dt}=\frac{q_c}{V}\left(c_c-\frac{\rho_c}{\rho}c\right)-\frac{q_w c}{V},\quad V=hA \tag{2}$$

A, the cross-sectional area of the tank, ρ_c and ρ, the inlet-brine and inlet-water/outlet-stream densities (respectively), and c_c, the inlet-brine concentration, are constant valued parameters in the model.

An example of the Simulink window built by students is shown in Figure 3. Furthermore, Matlab with Simulink can be used to compare the results of the first-principles nonlinear model with the responses obtained from its linearized equivalent at an operating condition; this enables students to evaluate the modeling errors associated with linearization.

Semiphysical modeling

The derivation of the semiphysical model follows along the line of the analysis presented in Lindskog.[6] Assuming constant volume in the tank (as the result of tight level control in the system) and constant densities for all streams, the first-principles model per Eqs. (1) and (2) reduces to

$$\frac{dc}{dt}=\frac{q_c c_c}{V}-\frac{(q_c+q_w)\,c}{V} \tag{3}$$

Using a forward-difference approximation on the derivative (for a sampling time T) leads to

$$\frac{c(t+T)-c(t)}{T}=\frac{q_c(t)c_c(t)}{V}-\frac{\left(q_c(t)+q_w(t)\right)c(t)}{V} \tag{4}$$

which solving for c(t+T) yields

$$c(t+T)=c(t)\frac{q_c(t)\,c_c(t)T}{V}-\frac{\left(q_c(t)+q_w(t)\right)c(t)T}{V} \tag{5}$$

Rearranging and consolidating terms, as well as renaming time in terms of sampling instants (t = k T, where k, the sampling instant, is an integer) leads to the semiphysical model structure

$$c(k)=c(k-1)+\theta_1 q_c(k-1)c_c(k-1)+\theta_2 q_c(k-1)c(k-1)+\theta_3 q_w(k-1)c(k-1) \tag{6}$$

Estimates of θ_1, θ_2, and θ_3 can be obtained from the first-principles model

$$\theta_1=\frac{T}{V}\qquad \theta_2=-\frac{T}{V}\qquad \theta_3=-\frac{T}{V} \tag{7}$$

or alternatively, they can be estimated from plant data by recognizing that θ_1, θ_2, and θ_3 are linear in the parameters and hence linear regression can be readily applied. The latter represents the semiphysical parameter estimation problem which can be easily computed in software packages widely available to students, such as Excel or Matlab.

A COMPREHENSIVE SEMIPHYSICAL MODELING EXPERIENCE

Having recognized that parameter estimation in semiphysical modeling constitutes a regression problem, students are then asked to perform a series of tasks that comprise a comprehensive identification procedure. These include:

The main objective of this experiment is to develop — via first principles and semiphysical modeling techniques — <u>useful</u> mathematical models of the tank behavior displaying good predictive ability.

> ***"All models are wrong, but some are useful."***
>
> —attributed to Prof. G.E.P. Box of the University of Wisconsin

1. ***Experimental Design.*** Students are asked to use the first-principles Matlab/Simulink model to design an informative experiment on the system. The design consists of a series of step changes of varying magnitude and duration that are intended to highlight the nonlinear behavior of the system and take into account the dominant time dynamics. The experiment must not exceed a two-hour time period (the length of a recitation session) and must avoid taking the sensors and actuators past their limits. Figure 4 shows a TDC3000 data screen for a typical experimental run designed by the students. Various experimental runs are performed over two weeks in the semester, and these are used to serve as estimation and validation data sets for the ensuing parameter-estimation problem.

2. ***Model structure selection and parameter estimation.*** Students are then asked to develop a Matlab program that uses regression analysis to estimate parameters of the semiphysical model. In addition to the three-parameter model structure shown in Eq. (6), the program must also estimate parameters for the following difference equation model structures, which are simple extensions to the model per Eq. (6):

Four-parameter model (Version A):

$$c(k)=\theta_4 c(k-1)+\theta_1 q_c(k-1)c_c(k-1)+\theta_2 q_c(k-1)c(k-1)+\theta_3 q_w(k-1)c(k-1) \quad (8)$$

Four-parameter model (Version B):

$$c(k)=c(k-1)+\theta_1 q_c(k-1)c_c(k-1)+\theta_2 q_c(k-1)c(k-1)+\theta_3 q_w(k-1)c(k-1)+\theta_4 \quad (9)$$

Five-parameter model:

$$c(k)=\theta_4 c(k-1)+\theta_1 q_c(k-1)c_c(k-1)+\theta_2 q_c(k-1)c(k-1)+\theta_3 q_w(k-1)c(k-1)+\theta_5 \quad (10)$$

The "four-parameter" and "five-parameter" models have more degrees of freedom and therefore allow greater flexibility in improving the goodness-of-fit as compared to the "three-parameter" difference equation.

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Four Parameter Model - Ver A
Estimated Theta1  = 0.019993
First principles, Theta1 = 0.013557

Estimated Theta2  = 0.047278
First principles, Theta2 = -0.014069

Estimated Theta3  = -0.015284
First principles, Theta3 = -0.013557

Estimated Theta4  = 0.98189
First principles, Theta4 = 1

Estimation Data Results
RMS error = 0.022619
MAX error = 0.056326

Validation Data Results
RMS error = 0.22734
MAX error = 0.46546
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Figure 6. *Parameter estimates for the four-parameter semiphysical model (Version A), compared with coefficients from first principles.*

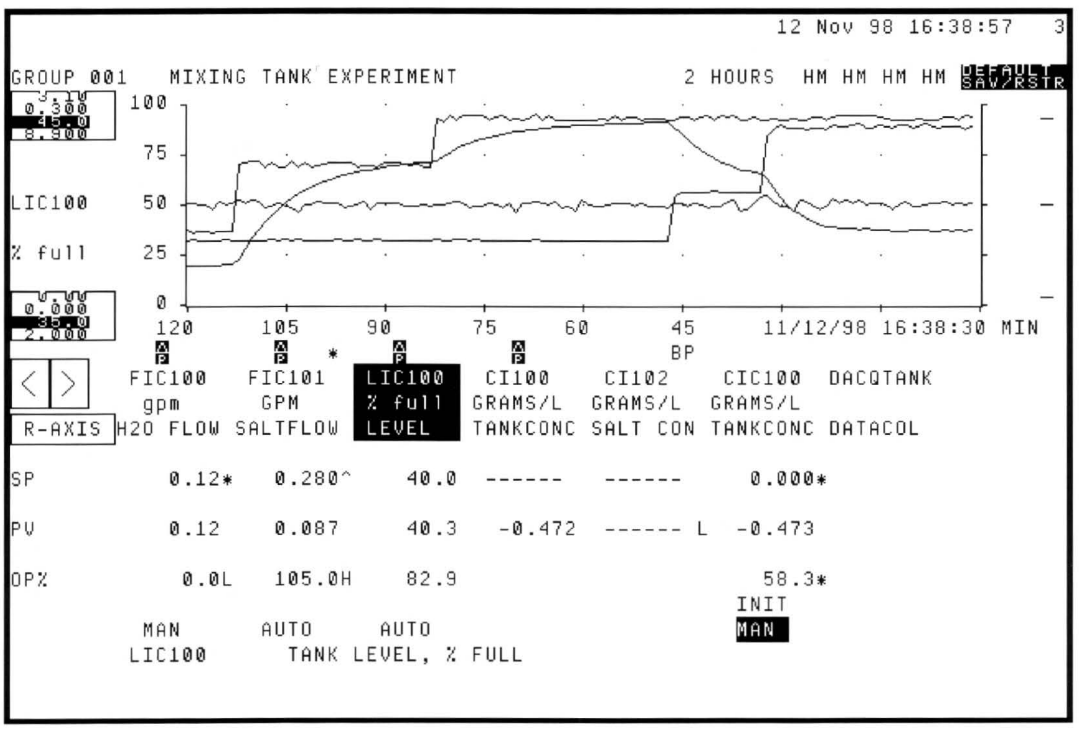

Figure 4. *Estimation data collected from the mixing tank, shown on a Honeywell TPS group display.*

3. ***Model Validation.*** Ultimately, the goal of model validation is to determine the model structure and parameters leading to predictions that are both physically meaningful and result in lower errors when compared on a validation data set (*i.e.*, a data set other than the one used for estimation). The semiphysical model estimates are compared against each other and against the responses obtained from the first-principles model (in both continuous-time and difference-equation form). In addition, students are asked to compute, display, and plot the maximum and root-mean-square (RMS) errors for both the estimation and cross-validation data sets. The RMS and maximum errors are determined on the basis of the residual time series

$$e_{resid}(k) = c(k) - \hat{c}(k), \quad k = 1, \cdots, N \tag{11}$$

which is the difference between the measured concentration ($c(k)$) and that estimated from a model ($\hat{c}(k)$). N is the total number of observations in the data set. The RMS error is computed as

$$RMSerr = \left(\frac{1}{N} \sum_{k=1}^{N} e_{resid}^2(k) \right)^{1/2} \tag{12}$$

while the maximum error consists of the largest absolute magnitude in the residuals,

$$MAXerr = \max_k \left| e_{resid}(k) \right|, \quad k = 1, \cdots, N \tag{13}$$

4. ***Reflection.*** Determining which model (semiphysical or first-principles) is "best" is not enough. Students are asked to examine their experience with the system and list all possible sources of error and prioritize them in order of importance. The inquisitive student will recognize problems related with the calibration of measurements, the relative effect of the simplifying assumptions, and similar circumstances. Ultimately, the students realize the importance of semiphysical modeling and of working with data as a valuable tool in modeling.

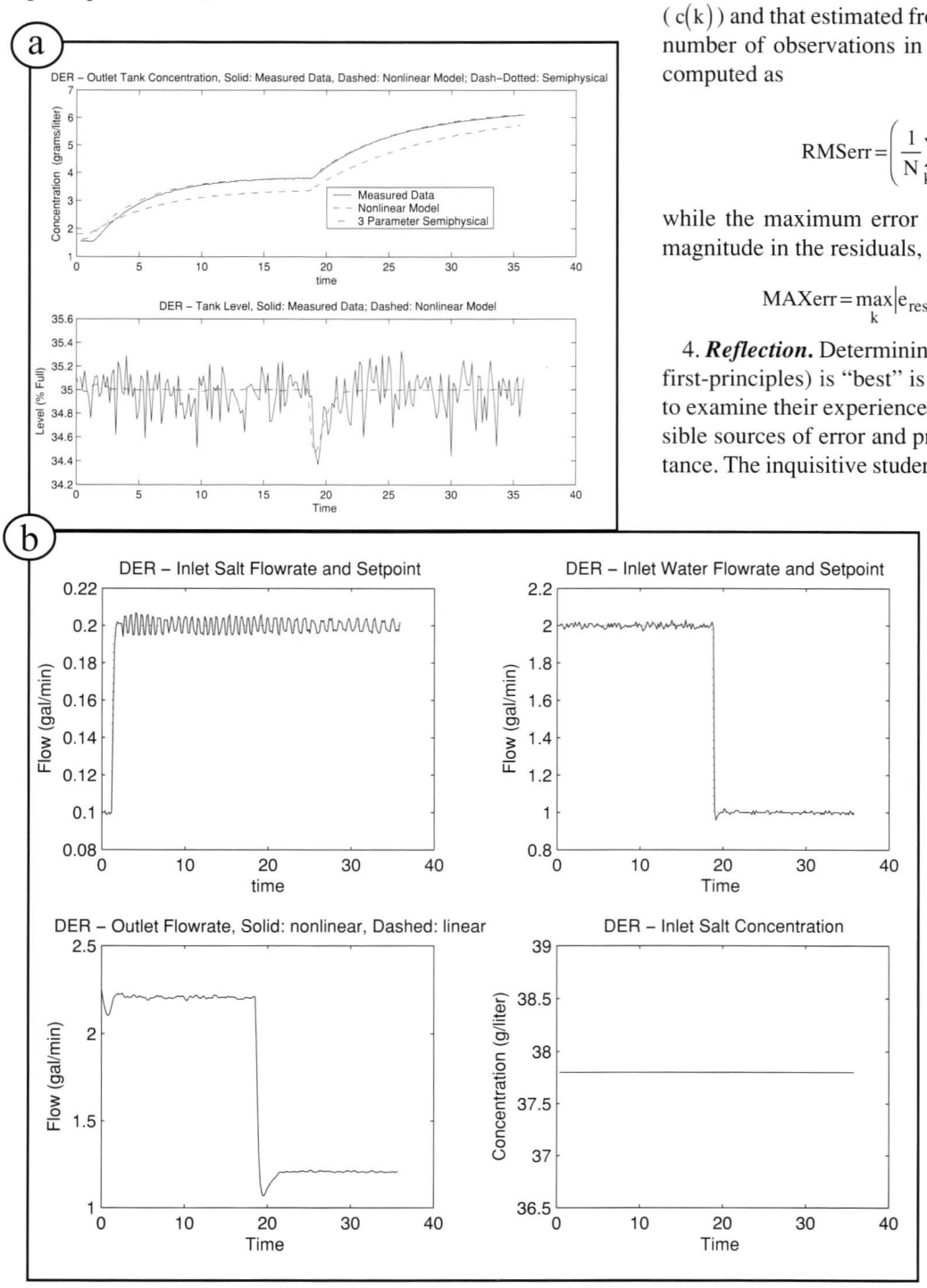

Figure 5. *Output* ***(a)*** *and input* ***(b)*** *time series for the estimation data set.*

An illustration of the various steps with some representative test data sets is shown in Figures 5 through 8. These plots are generated using the Matlab/Simulink files developed by the students over the course of the semester. A typical estimation data set (consisting in this case of one step change each for the inlet brine and freshwater flows) is shown in Figure 5. Parameter estimates are presented on the Matlab command window and compared to first-principles coefficients; Figure 6 shows typical values obtained for the four-parameter model (Ver-

sion A). Simulation results on the estimation and validation data sets that include the first-principles model, and the regression results using the various semiphysical model structures presented earlier, are shown in Figure 7. There is relative agreement between the first principles and three-parameter semiphysical model results, as can be seen in Figure 6. All semiphysical models closely agree (Figure 7a), and as reflected by the RMS values (Figure 8a), increasing the number of parameters yields improved goodness of fit in the estimation data set. Simulation results on the validation data set seen in Figure 7b, however, indicate that the four-parameter model (Version A) has the best predictive ability over all the evaluated models; this is ultimately the most important criterion in discriminating between the various models. Besides a better visual fit in the simulation, the four-parameter model (Version A) also displays superior RMS (Figure 8b) and MAX errors (not shown).

STUDENT FEEDBACK AND ASSESSMENT

Prior to the introduction of the brine-water mixing tank experiment in ECE 394 Systems, student exposure to real-time data acquisition and measurement was minimal (until the senior year, when they were required to take ChE 461, Process Dynamics and Control). Likewise, Matlab experience was limited to working with M-functions in a core numerical methods course (ECE 384), and there was no exposure to Simulink. As a result, much of the strongest praise and recognition of the benefits of the ECE 394 Systems course was offered by students during their senior year, or following employment in industry or graduate school (as evidenced by many anecdotal experiences shared with the instructor). Nonetheless, student evaluation responses to the question "What did you like the most about the course?" often focused on the recitation/lab experience involving the brine-water mixing tank experiment. Some comments include:

- *"I liked the opportunity to get hands-on experience in the lab. It was fun learning how to use Matlab and Simulink to model what was going on in class. Also, I believe this class will prepare me quite well for others."*
- *"I was able to relate course material to real-world problems . . . . I felt like I learned a lot."*
- *"(I liked) the fact that near the end of the course the theoretical parts of the course were shown in a practical way, i.e., working with the mixing tank."*
- *"Going to work with the brine-water tank reinforced what we did in class. Usually you do not get to apply what you learn in a class, but our lab gave us this opportunity."*

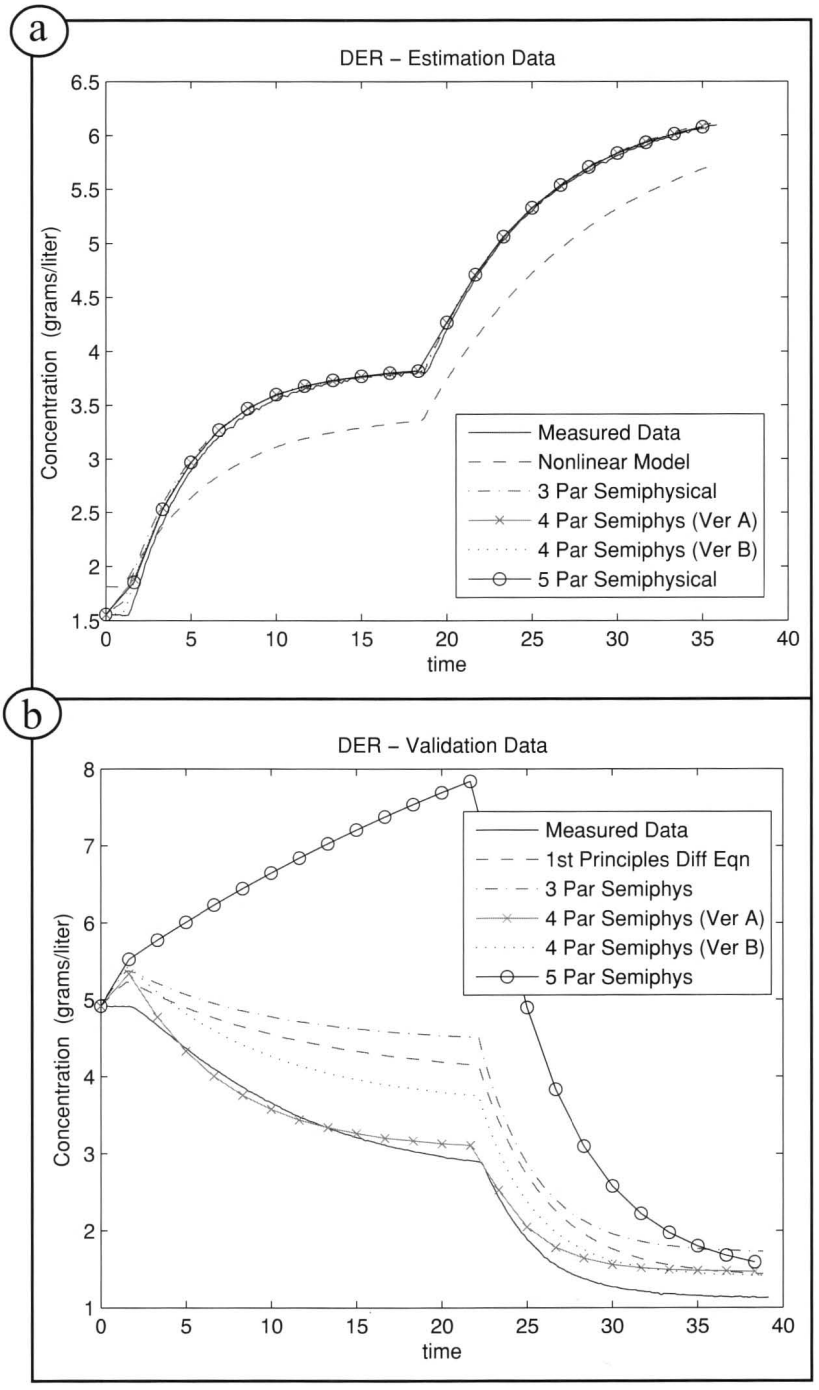

Figure 7. *Simulation results on the estimation* ***(a)*** *and validation* ***(b)*** *data sets for the first-principles and semiphysical models.*

- *"The recitation period was very different and interesting . . . it made us think!"*
- *"The projects and lab materials were the best part of the course. They gave me the chance to see actual uses for my degree."*

Student criticism associated with the brine-water experiment consisted principally of complaints on the perceived additional workload created by project, as well as the timing of the final project report (which some students felt was too close to finals). One student requested that peer assessment be part of the final project grade. Some criticism was particularly noteworthy, for instance:

- *"There was, perhaps, too much computer modeling done in this course. I did, however, enjoy doing it."*

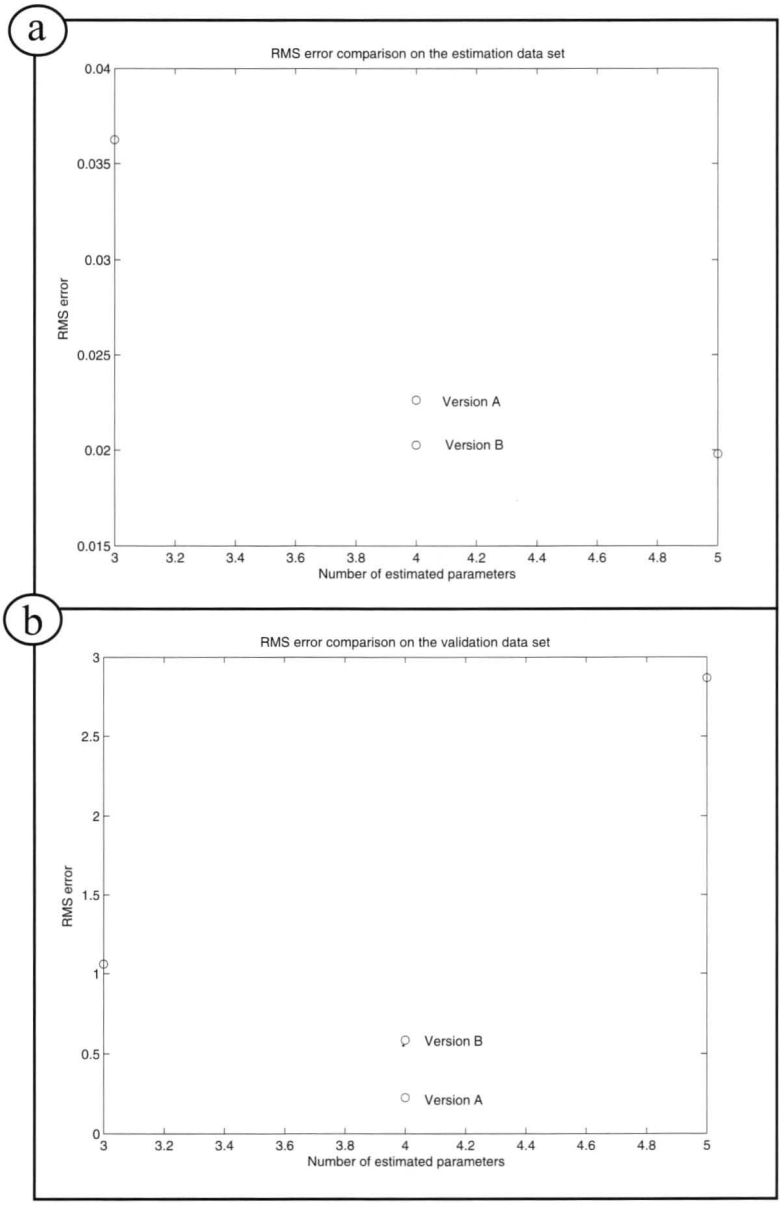

Figure 8. *RMS error comparison on the estimation* ***(a)*** *and validations* ***(b)*** *data sets.*

SUMMARY AND CONCLUSIONS

The brine-water mixing tank is a relatively simple experiment that can be readily taught to students across disciplines. The experiment described in this paper exposes students to significant concepts in dynamical modeling, system identification, and numerical computing in a challenging experimental and real-time information setting. Semiphysical modeling is introduced in a meaningful way while demanding only a modest mathematical background from students: knowledge of differential equations, basic numerical methods, and regression analysis. Aside from a dedicated engineering systems course, this experiment can serve an important role in either an introductory process dynamics and control course or a senior-level unit operations laboratory. Copies of the Matlab/Simulink files implementing this procedure, including some sample data files, can be obtained by request from the author via e-mail (daniel.rivera@asu.edu).

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